National Center for Computational Sciences Snapshot
The Week of February 19, 2007

Vis Experts Gather in Salt Lake City

As the world's fastest computers reach levels of power once unimaginable, researchers find they must make sense of a growing mountain of data.

Fortunately they have allies among visualization experts—such as members of the National Center for Computational Sciences' (NCCS's) visualization team—who are able to take data and convert it into images and movies that make sense of the information.

The Department of Energy's Scientific Discovery through Advanced Computing (SciDAC) program also recognizes the importance of visualization. In response it has created the Visualization and Analytics Center for Enabling Technologies (VACET), a collaboration of visualization and data-analysis professionals from institutions around the country, and the SciDAC Institute for Ultrascale Visualization at the University of California (UC)–Davis.

Created in 2006, VACET held its first all-hands meeting this month in Salt Lake City, giving visualization researchers an opportunity to get together and brainstorm as well as to match SciDAC projects with the proper tools.

"VACET is a center for helping SciDAC application scientists get meaning out of their data," explained Sean Ahern, who is the NCCS visualization team leader and serves as Oak Ridge National Laboratory's (ORNL's) principal investigator for the center. "We have everything from small data sets that are fairly complex all the way out to incredibly large problems."

The center comprises visualization experts from five institutions. Besides ORNL, members come from Lawrence Livermore and Lawrence Berkeley national laboratories, the University of Utah, and UC–Davis. Ahern attended the meeting with Jamison Daniel, also of the NCCS visualization team, and George Ostrouchov and Jeremy Meredith from ORNL's Computer Science and Mathematics Division (CSM).

"While the executive committee has met several times, this is the first time that we have had everybody in the project come together in one place to talk about the technologies," Ahern explained. "It was very useful to get everybody together.

"You can certainly have some level of communication by e-mail and teleconferences, but actually getting everybody in the same room so you can have little spinoff groups talking about various technologies, it's a very rich environment in which to develop collaborations. It's the collaborations that will decide whether this project sinks or swims."

One important aspect of the meeting was matching projects with the data-analysis tools that would serve them best.

“We had application scientists come and talk to us—either through teleconference or in person—about their needs,” Ahern explained, “and then we did a match between the technologies and their needs. That was its central core.”

The center works to develop tools that present increasing levels of information with increasing flexibility. For example, members are working on technology that is able to convey high-dimensional data sets, which give many pieces of information about each point in the simulation.

The center is also looking at other ways of analyzing the data. Ahern noted that Ostrouchov of CSM is a statistician rather than a visualization expert.

“There are many techniques in the area of statistical analysis that we can borrow to be able to extract meaning,” he noted. “For example, when we’re attempting to view 40 billion particles, there are a lot of techniques in statistics that allow us to describe the aggregate behavior of particles without having to describe the behavior of each individual one.”

Members of the ORNL team are no strangers to developing and improving data-analysis tools. While at Lawrence Livermore National Laboratory, Ahern and Meredith were among the principal developers of VisIt, a major visualization tool that now has thousands of users across the world. Among his contributions, Ahern designed the program’s ability to derive new variables from ones that were included in the original simulation.

“The ability to do on-the-fly analysis is what I designed,” he said. “I’m pretty proud of that; it’s a fairly powerful part of the tool.”

XT4 Open for Business

Jaguar users recently got a 20 percent boost in computing power with the acceptance of the 68-cabinet Cray XT4 on the second floor of the NCCS.

Last week users were moved from the XT3 system on the first floor to the new XT4 system. The newer system boasts a peak performance of 65 trillion floating-point operations per second (65 teraflops), compared to a peak performance of 54 teraflops for the older system.

The 56 XT3 cabinets have now been moved to the second floor as well, and the two systems will be connected and ready for use by the end of March, creating a system with a peak performance of 119 teraflops.

Eventually the system will be upgraded to a peak performance of 250 teraflops as the dual-core processors are replaced with quad-core processors in the XT4 cabinets.

Distance Lectures Introduce ORNL Experts to Georgia Tech Students

Students at the Georgia Institute of Technology have an opportunity this semester to spend their Friday afternoons learning about computing from the experts at ORNL.

Thomas Zacharia, Associate Laboratory Director for the Computing and Computational Sciences Directorate and an adjunct professor for The University of Tennessee's College of Engineering, is leading the distance lecture series in his role as a member of Georgia Tech's faculty. The series involves lectures each Friday held at the Joint Institute for Computational Sciences auditorium on the ORNL campus and broadcast to students at Georgia Tech.

The speakers include Zacharia, who presented an introduction to ORNL, and Leadership Computing Facility Director Buddy Bland, who will discuss facilities for high-performance computing. Other speakers and the topics they will speak on include

- Bronson Messer of the NCCS, "Computational Astrophysics";
- Brian Worley of the Computational Sciences and Engineering Division (CSE), "Knowledge Discovery";
- Sean Ahern, visualization team leader at the NCCS, "Visualization for HPC";
- Arjun Shankar of CSE, "Computational Techniques for Smart Electric Grids";
- Richard Bass of CSE, "Advanced Modeling and Computation for Nuclear Safety and Reliability";
- Scott Studham of the Office of the Chief Information Officer, "IT and Cybersecurity at ORNL";
- Kalyan Perumalla of CSE, "HPC and Data-Enabled Solutions for Critical Applications";
- Ramanan Sankaran of the NCCS, "Combustion Modeling";
- Budhu Bhaduri of CSE, "Geographic Information Science";
- Ryan Bennink of CSE, "The New Science and Quantum Information"; and
- Victor Hazlewood of the Office of the Chief Information Officer, "Cybersecurity."